K.L.University
Vaddeswaram- 522502
M.Sc., General Chemistry, II-Semester, 2016-17

Course Handout

1. Course Name : General Chemistry

2. Course Code : 16CY 1205

3. Course Coordinator : Dr. T Bhaskara Rao

4. Course Structure(LTP) :

L	T	P
4	0	0

5. Credits : 4

6. Team Members : Dr. N. V Suresh Kumar

Course Description: "General chemistry is the science that systematically studies the composition, properties, and activity of organic and inorganic substances and various elementary forms of matter."

Course Objectives:

Provide in-depth understanding on the Organic and Inorganic structure determination of chemical substances using few spectroscopic techniques .To gain fundamental knowledge in crystal structures, Spectroscopy and its application. Analytical skill development for their future career in both research and industry.

7. Upon completion of the course, students will:

CO	CO	BTL
I	Symmetry and Group theory of the molecules	2
II	Energy associates with the degrees of freedom	2
III	Classical and quantum theories of Raman and Electronic Spectra of diatomic molecules and poly atomic molecules	2
IV	Basic principles and Applications of Nuclear Magnetic Resonance Spectroscopy	2

8. Course outcome Indicators:

CO#	COI-1	COI-2	COI-3
CO-I	Understand the Symmetry, operation and relation between order of a finite group	Describe the Point symmetry group	Describe the theorem and applications of groups theory
CO-II	Type of spectra Microwave spectroscopy and Classification of molecules	Describe vibrational energies of diatomic molecules and zero point energy	Application IR to structure elucidation of organic molecules
CO-III	Explain Classical and quantum theories of Raman effects	Understand the concept of Visible and ultraviolet spectroscopy	Describe the fine structure of electronic vibrational transition
CO-IV	Understand the magnetic properties of molecules	Discuss the principal and theory of NMR Spectroscopy	Basic ideas about instrument NMR studies of nuclei other than proton

9. Program Outcomes (Pos):

PO1. Apply knowledge of mathematics, science, engineering fundamentals and an engineering specialization to the conceptualization of engineering models.

PO2. Identify, formulate, research literature and solve complex engineering problems reaching sustained conclusions using first principles of mathematics and engineering sciences.

PO3. Design solutions for complex engineering problems and design systems, components or processes that meet specified needs with appropriate consideration for public health and safety, cultural, societal and environmental considerations.

PO4. Conduct investigations of complex problems including design of experiments, analysis and interpretation of data and synthesis of information to provide valid conclusions.

PO5. Create, select and apply appropriate techniques, resources and modern engineering tools including predictions and modeling, to complex engineering activities, with an understanding of the limitations.

PO6. Function effectively as an individual, and as a member or leader in diverse teams and in multi disciplinary settings.

PO7. Communicate effectively on complex engineering activities with the engineering community and with society at large, such as being able to comprehend

and write effective report and design documentation, make effective presentation, give and receive clear instructions.
PO8. Demonstrate understanding of societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to engineering practice.

PO9. Understand and commit to professional ethics and responsibilities and norms of engineering practice.

PO10. Understand impact of engineering solutions in a societal context and demonstrate knowledge of and need for sustainable development.

PO11. Demonstrate a knowledge and understanding of management and business practice, such as risk and change management, and understand their limitations.

PO12. Recognize the need for, and have the ability to engage in independent and lifelong learning.

10. Mapping of Course Objectives with Programme Outcomes:

1. Highest 2. Moderate 3. Use

Programme Outcomes (Pos)												
Course Out come	**P01**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**	**PO11**	**PO12**
CO-I		1	1	1	2	1	2		1		3	1
CO-II		1	1	1	2	1	2		1		3	1
CO-III		1	1	1	2	1	2		1		2	1
CO-IV		2							2			

11. Time Table:

Day/Time	9.00-9.50	9.50-10.40	10.50-11.40	11.50-12.40	01:00 -04:00
Monday					
Tuesday					
Wednesday	Dr NSK				
Thursday		Dr TBR			
Friday			Dr NSK		
Saturday	Dr TBR				

12. Syllabus:

UNIT-1
Symmetry and Group theory in Chemistry - Symmetry elements, symmetry operation, definition of group, suib group, relation between order of a finite group and its sub group. Point symmetry group. Schonfiles symbols, representation of groups by Matrices (representation for the Cn, Cnv, Cnh, Dn etc.groups to be worked out, explicitely). Character of a representation. The great orthogonality theorem(without proof) and its importance. Character tables and their use. Application of group theory in IR and Raman spectroscopy.
UNIT – II
Motion of molecules-Degrees of freedom –Energy associates with the degrees of freedom Type of spectra Microwave spectroscopy. Classification molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, Intensities non-rigid rotator-Microwave spectra of polyatomic molecules.Infared spectroscopy Harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths, anhoremonicity Morse potential energy diagram. Vibration – rotation spectroscopy. PQR braches, Born – oppenheimer approximation, Break down Born – openheimer approximation, selectionrules, normal modes of vibration group frequencies, overtones, hot bands, application of IR spectra topolyatomic molecules.
UNIT – III
Raman spectroscopy. Classical and quantum theories of Raman effects, pure rotational, vibrational and Vibrational – rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent antistrakes Raman Spectroscopy (CARS) – Application.Visible and ultraviolet spectroscopy: - Electronic Spectra of diatomic molecules, vibrational structure ofan electronic transition, classification of bands, rotational fine structure of electronic vibrational transition. Electronic Spectra of Polyatomic Molecules – Instrumentation – Applications.
UNIT – IV
Nuclear Magnetic Resonance Spectroscopy: - Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, desheilding, spin – spin interactions, factors influencing, coupling constant J. Classification (ABX, AMX, ABC, A2, B2 etc.) Basic ideas about instrument NMR studies of nuclei other than proton – $_{13}C$,$_{19}F$, $_{31}P$. Use of NMR in medical diagnostics.
SUGGESTED BOOKS:
1.Fundamentals of Molecular spectroscopy: by C.N.Banwell
2.Introductory Group Theory for Chemists – George Davidson
3.Group theory for chemistry – A.K.Bhattacharya
4.Molecular spectroscopy by B.K.Sharma
5. Vibrational Spectroscopy by D.N.Sathyanarayana New Age Int. Pub.
6. Spectroscopy by Aruldas.
7.Chemical Analysis by H.A.Laitinan and W.E.Harris, McGraw Hill.

13. Self Learning Topics:

CO	Topic	Source
I	representation of groups by Matrices (representation for the Cn, Cnv, Cnh, Dn etc	T-1
II	Infared spectroscopy Harmonic oscillator,	T-1
III	coupling constant J. Classification (ABX, AMX, ABC, A2, B2 etc.)	T-1
IV	Basic ideas about instrument NMR studies of	Internet Sources
V	nuclei other than proton – $_{13}C$,$_{19}F$, $_{31}P$. Use of NMR in medical diagnostics	Internet Sources

14.Session / Lesson Plan

S. No	CO	Session	Content and Source	Learning objective, End of the session student will	Teaching Methodology	Faculty Approach	Student Approach	Cognitive level expected
1	I	1	Symmetry elements, symmetry operation	Understand the necessity	Oral	Explanation	Listens and participate	Understand
2	I	2	definition of group, suib group	Understand	Chalk and talk	Explanation	Listens and participate	Understand
3	I	3	relation between order of a finite group and its sub group	Understand	Chalk and talk	Explanation	Listen	Understand
4	I	4	Point symmetry group. Schonfiles symbols	Apply and use	Chalk and talk	Explanation	Listen and Practice	Understand And apply
5	I	5	groups to be worked out, explicitely).	Understand	Chalk and talk	Explanation	Listen and Practice	Understand And apply
6	I	6	groups to be worked out, explicitely).	Understand	Chalk and talk	Explanation	Listen and	Understand
7	I	7	Character of a representation.	Understand	Chalk and talk	Explanation	Listen	Understand
8	I	8	The great orthogonality theorem(without proof) and its importance	Understand	Chalk and talk	Explanation	Listen	Understand
9	I	9	The great orthogonality theorem(without proof) and its importance	Understand	PPT	Explanation	Listen	Understand
10	I	10	Character tables and their use	Apply and use	PPT	Explanation	Listen	Apply and use
11	I	11	Application of group theory in IR and Raman spectroscopy.	Apply and use	Chalk and talk	Explanation	Listen and practice	Apply and use
12	I	12	Application of group theory in IR and Raman spectroscopy.	Apply and use	Chalk and talk /PPT	Explanation	Listen	Apply and use
13	II	13	Motion of molecules-Degrees of freedom	Understand	Chalk and talk / PPT	Explanation	Listen and analyze	Understand
14	II	14	Energy associates with the degrees of freedom	Understand	Chalk and talk	Explanation	Listen	Understand
15	II	15	Type of spectra Microwave spectroscopy	Understand	Chalk and talk	Explanation	Listen	Understand And remember
16	II	16	Classification molecules, rigid rotator model,	Understand	Chalk and talk	Explanation	Listen	Understand And remember

17	II	17	effect of isotopic substitution on the transition frequencies,	Analyze	Chalk and talk /PPT	Explanation	Listen and practice	Analyze
18	II	18	Intensities non-rigid rotator-Microwave spectra of polyatomic molecules	Analyze	Chalk and talk	Explanation	Listen and practice	Analyze
19	II	19	vibrational energies of diatomic molecules, zero point energy,	Understand, Analyze	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
20	II	20	force constant and bond strengths, anhoremonicity Morse potential energy diagram. Vibration –	Understand, Analyze	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
21	II	21	rotation spectroscopy. PQR braches, Born – oppenheimer approximation, Break down Born	Understand	Chalk and talk / PPT	Explanation	Listen	Understand
22	II	22	openheimer approximation, selectionrules, normal modes of vibration group frequencies,	Understand	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
23	II	23	overtones, hot bands, application of IR spectra topolyatomic molecules.	Analyze	Chalk and talk	Explanation	Listen and practice	Analyze
24	III	24	Raman spectroscopy. Classical and quantum theories of Raman effects	Analyze	Chalk and talk	Explanation	Listen	Analyze
25	III	25	pure rotational, vibrational and Vibrational – rotational Raman spectra, selection rules, mutual exclusion principle,	Apply and use	Chalk and talk / PPT	Explanation	Listen	Apply and use
26	III	26	Resonance Raman spectroscopy, coherent antistrakes Raman Spectroscopy (CARS)	Apply and use	Chalk and talk / PPT	Explanation	Listen	Apply and use
27	III	27	Application.Visible and ultraviolet spectroscopy:	Understand	Chalk and talk	Explanation	Listen and participate	Understand
28	III	28	Electronic Spectra of diatomic molecules, vibrational structure ofan electronic transition	Apply and use	Chalk and talk	Explanation	Listen and participate	Apply and use
29	III	29	Electronic Spectra of diatomic molecules, vibrational structure ofan electronic transition	Apply and use	Chalk and talk	Explanation	Listen	Apply and use
30	III	30	classification of bands, rotational fine structure of electronic vibrational	Understand	Chalk and talk	Explanation	Listen and participate	Understand

			transition.					
31	III	31	classification of bands, rotational fine structure of electronic vibrational transition.	Understand	Chalk and talk	Explanation	Listen	Understand
32	III	32	Electronic Spectra of Polyatomic Molecules – Instrumentation – Applications.	Understand	Chalk and talk	Explanation	Listen	Understand
33	III	33	Electronic Spectra of Polyatomic Molecules – Instrumentation – Applications.	Understand	Chalk and talk	Explanation	Listen	Understand
34	IV	34	Introduction of Nuclear Magnetic Resonance Spectroscopy					
35	IV	35	, Nuclear spin, nuclear resonance,					
36	IV	36	, saturation, shielding of magnetic nuclei					
37	IV	37	chemical shift and its measurements,					
38	1V	38	factors influencing chemical shift, desheilding,					
39	1V	39	spin – spin interactions					
40	IV	40	factors influencing					

15. **Evaluation scheme:**

EVALUATION PLAN FOR COURSES (16CY110-organic chemistry)

Evaluation Component	Marks	Weightage	Date	Duration (Hours)	CO 1		CO 2		CO 3		CO 4	
	Course Outcome Indicator Number				1	2	1	2	1	2	1	2
	Blooms Taxonomy Level				1	2	2	2	2	2	1	2
Assignment Test	20	5 %		1 ½	10	10						
Test 1	20	20%*		1 ½			10	10				
Test 2	20			1 ½					10	10		
Home Assignment	20	5%		-							10	10
Quiz	20	5%		20 min	5		5		5		5	
Attendance	5	5%	----		75% of Theory+25% of lab attendance.							
Semester End Exam	60	60%		3	2	10.5	2	10.5	2	10.5	2	10.5
					3	12	3	12	3	12	3	12

*** 75 % of the Best and 25% of other test together will be taken for 20 marks, internal.**

TEST PATERN:

1. **Assignment Test**: 6 Questions will be given in advance and any two questions of the Faculty choice have to be answered.
2. **TEST1 & 2**: It comprises two sections: **Section-1**: 6 short answer question of 1 mark each are to be answered (no choice). **Section-2**: 2 questions of 7 marks each out of 3 questions have to be answered, totaling to 20 marks. **75 % of the Best and 25% of other test together will be taken for 20 marks, internal.**
3. **Home Assignment**: Two Questions will be given for 10 marks each and to be submitted on or before submission date announced by the faculty in the class.
4. **Quiz:** 20 Objective Questions will be given for 10 marks and to be answered in 20 minutes.
5. **Semester End exam**: Four questions with internal choice 4x15=60

Chamber consultation hours: Saturday: 12:40 PM- 2:20PM

Tuesday: 12:40 PM- 2:20PM

16. Notices:

All notices regarding course matters will be displayed in e-learning site & copy of it in department notice board.

Note:

a. Each student is required to attend all classes regularly with calculator and is required to complete all the work assigned for the course.
b. Instructors of courses are not obligated to provide make-up opportunities for students who are absent, unless the absence has been officially approved. An

officially approved absence, however, merely gives the individual who missed the class an opportunity to make up the work and in no way excuses him from the work.

c. Re conduction of tests will not be entertained, whatever may be the reason. Submission of home assignments after the deadline will not be either accepted or awarded any marks.
d. All students in the class must treat others with civility and respect and conduct themselves during class sessions in a way that does not unreasonably interfere with the opportunity of other students to learn. Failure to comply with this requirement may result in points being deducted from a student's final numerical average / soft skills.

17. Signature of the Course Coordinator:

18. Signature of the Group Head:

19. Signature of the HOD: